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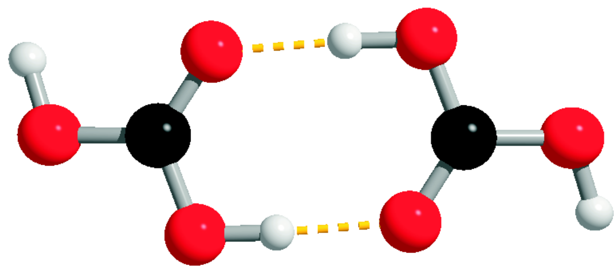

Despite the conventional wisdom that carbonic acid is kinetically instable, chemists recently succeeded in recognizing its stability and then in isolating and characterizing this compound. In particular, Hage et al. [1] were able to sublime and recondense carbonic acid without decomposition into carbon dioxide and water. This study could prove the stability of gas-phase carbonic acid. The vapor pressure estimates were consistent with an equilibrium mixture of monomers and dimers, comparable to that of formic acid. In this work we use the recently developed quantum cluster equilibrium (QCE) theory [2,3] at the RHF/6-31+G$*$ and at the B3LYP/6-31+G$*$ level of theory to calculate the equilibrium cluster population for carbonic acid in the gas and the solid phase. The validity of the resulting QCE model is tested by comparison with experimental thermodynamic and spectroscopic data.

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